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United Technologies Research Center
East Hartford, CT 06108

June 1981

Prepared for
NATIONAL AERONAUTICS AND SPACE ADMINISTRATION
Lewis Research Center
Under Contract NAS3-20066

for
**U.S. DEPARTMENT OF ENERGY
Conservation and Solar Energy
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FOREWORD

The work reported herein was performed at the United Technologies Research Center (UTRC), East Hartford, Connecticut, for the U. S. Department of Energy (DOE) under Contract NAS3-20066. The program was conducted under the technical management of Mr. R. R. Tacina of the NASA-Lewis Research Center, Cleveland, Ohio, as a part of the DOE Gas Turbine Highway Vehicle Systems Program. Dr. L. J. Spadaccini was the UTRC Program Manager.

Autoignition Characteristics of No. 2 Diesel Fuel

John A. TeVelde
Louis J. Spadaccini

SUMMARY

An applied research program was undertaken to evaluate the autoignition characteristics of No. 2 diesel fuel in air over ranges of air temperature, pressure and equivalence ratio appropriate to regenerative-cycle automotive gas turbine engines. Ignition delay times were measured using a continuous flow test apparatus which enables the independent variation and evaluation of the effects of temperature, pressure, and fuel-air ratio on ignition delay times over the range of conditions of interest.

Parametric tests to map the ignition delay characteristics of No. 2 diesel fuel were conducted at pressures of 3, 4, and 5 atm, inlet air temperatures up to 1150K and fuel-air equivalence ratios ranging from 0.2 to 1.0. Ignition delay times in the range of 6 msec to 60 msec at freestream flow velocities ranging from 10 m/sec to 40 m/sec were obtained. Similar to results reported in Ref. 1, the ignition delay times appeared to correlate with the inverse of pressure and the inverse exponent of temperature; viz:

$$\tau = A/P^n \exp(E/RT)$$

INTRODUCTION

Lean combustion of premixed/prevaporized fuel in gas turbine engines is a most promising approach for reducing NO_x emissions, improving durability and performance, and providing fuel flexibility. However, an intrinsic problem to be treated in the design of premixing/prevaporizing combustors is the potential for inadvertent autoignition of the fuel-air mixture prior to injection into the primary combustion zone. In regenerative-cycle automotive gas turbine engines the extremely high combustor inlet temperatures can easily promote ignition in the premixing passages, if the residence time is sufficiently long. Consequently, mixing and vaporization must be completed rapidly.

This program is an extension of earlier efforts (Ref. 1) which led to the successful development of a fundamental autoignition experiment and the comprehensive mapping of the ignition delay times of several liquid hydrocarbon fuels in air at conditions appropriate to aircraft gas turbine engines. The present extension comprises experimental efforts to map the ignition delay characteristics of No. 2 diesel fuel at temperatures and pressures which are representative of regenerative-cycle automotive gas turbine engines.

Previous Experimental Techniques

A great variety of equipment and procedures has been used to measure the ignition delay of liquid hydrocarbon fuels, including constant volume bombs, reciprocating engines and steady-flow test apparatus. However, the spontaneous ignition temperature of a combustible substance is not an absolute property of the substance and, consequently, all spontaneous ignition data need to be interpreted carefully in the light of the test apparatus and methods used for their determination. Existing experimental data are generally dependent on the particular experimental configuration employed and are, therefore, too inconsistent for universal design use.

An extensive survey and discussion of numerous early autoignition investigations can be found in Ref. 1. This survey served as a basis for formulating the present continuous flow experiment which was then developed and used to evaluate the autoignition characteristics of five liquid hydrocarbon fuels in air at conditions appropriate to advanced gas turbine engines. Ignition delay times in the range of 1 msec to 50 msec were obtained over freestream flow velocities ranging from 20 m/sec to 100 m/sec, pressures ranging from 10 atm to 30 atm, air temperatures ranging from 640K to 1000K and fuel-air ratios ranging from 0.3 to 1.0. The ignition delay times for all fuels tested were correlated according to the following Arrhenius-type equation

$$\tau = A/P^n \exp (E/RT)$$

where A, E and n are empirically derived constants, P is the air pressure, R is the universal gas constant, T is the inlet air temperature and τ is the ignition delay time.

More recently, Tacina (Ref. 2) measured the ignition delay characteristics of No. 2 diesel fuel in an insulated premixing/prevaporizing fuel preparation duct at conditions applicable to the automotive gas turbine engine. A range of inlet air temperatures from 600K to 1000K, equivalence ratios ranging from 0.13 to 1.05, air pressures ranging from 1.8 atm to 6.8 atm and freestream flow velocities from 3.5 m/sec to 30 m/sec were investigated. Although experiencing a considerable amount of data scatter, Tacina determined that for test section (mixing/vaporizing section) lengths from 16 to 48 cm, the correlation which best represented the data could be expressed as,

$$(p/V) \phi^{1.3} = 0.62 \exp (2800/T)$$

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where p is the pressure in kPa, V is the velocity in m/sec, ϕ is the equivalence ratio and T is the inlet temperature in degrees Kelvin.

There is considerable disagreement among the previous investigators regarding the importance of many of the dependent variables on autoignition. Some have reported no effect of mixture ratio, others a minor effect, and still others have found a major effect. Some have reported that ignition delay varies as the inverse square of pressure, others as simply the reciprocal of pressure, and still others report that ignition delay is even less sensitive to air pressure. These differences or inconsistencies underscore the previous admonition that ignition delay data need to be interpreted carefully in the light of the test apparatus and the methods used to identify the autoignition event.

EXPERIMENTAL APPROACH

Description of Apparatus

Parametric autoignition data pertinent to gas turbine engines can best be acquired by conducting a continuous flow experiment using dry, unvitiated air, and providing independent control of pressure, temperature, and air and fuel mass flow rates. The test apparatus developed in Ref. 1 and modified in the present program is shown in Fig. 1. It consists of (1) a 720 kW electric resistance-type air heater which is capable of heating the air stream to 925K, (2) an air bypass section that is necessary to satisfy the minimum flow requirements of the 720 kW heater, (3) a 20 kW high-temperature electric heater capable of raising the air temperature to 1200K, (4) a flow straightener, (5) a premixing-type fuel injector, (6) a cylindrical mixer/vaporizer section consisting of several flanged spool pieces which permit length variations over a range from 2.5 cm to 150 cm in increments of 2.5 cm, (7) an expander section which provides a sudden expansion and water quench at the autoignition station, and (8) a remotely operated throttle valve located in the exhaust ducting.

Details of the mixer/vaporizer and expander sections are shown in Fig. 2. The inner surface of the mixer/vaporizer sections are smooth and free of boundary discontinuities capable of producing wakes in the flow. This is accomplished by internal machining and the use of alignment dowels for each section of the mixer/vaporizer. The walls of the mixer/vaporizer sections were water cooled during all tests both to preserve the structural integrity of the apparatus and to preclude the possibility of ignition and flashback via the boundary layer. Water injection was provided at the step region to prevent flame stabilization at the exit of the mixer/vaporizer section. Thermocouples and photodetectors were used to monitor the step region and identify conditions which would result in flame stabilization.

Inlet air temperature and pressure were measured upstream of the fuel injection location. Choked venturis were used to measure both the total inlet airflow rate and the bypass airflow rate. The fuel flow rate was measured using a calibrated turbine meter. Fuel pressures were monitored at the injection station. The occurrence of autoignition was determined by (1) a thermocouple probe (located in the expander section), (2) photodetectors (located at several positions in the test rig), (3) a differential pressure transducer monitoring the pressure drop across the mixer/vaporizer section, and (4) an absolute pressure transducer in the mixer/vaporizer section (see Fig. 2).

Since the generation of a uniform fuel-air mixture in the shortest distance (time) possible is crucial for determining the effect of fuel/air ratio on autoignition, the multiple conical tube-type injector used in Ref. 1 was also used in this test program. This injector, shown in Fig. 3, consisted of a 19 hole concentric array of venturi-shaped air passages having throat diameters of 0.55 cm and with independently-controlled fuel injection into the converging section of each element using 0.084-cm ID tubing. Downstream recirculation zones were eliminated by extending the diverging sections of the venturis to the points of intersection, thereby eliminating a base region. Also, the relatively high blockage area (approximately 70 percent) acted to reduce inlet airflow nonuniformities. An earlier characterization of this injector (Ref. 1) with the center and outer elements capped resulted in a nearly uniform profile at radial positions up to $R/R_o = \pm 0.5$ and also minimized fuel accumulation along the walls. Therefore, the same configuration (i.e., center and outer elements capped) was used in the present program. The fuel pressure drop across the injector orifices varied between 5 and 50 psi, depending on the fuel flow rates tested. However, because the fuel and air flow rates in the present program are considerably different from those of Ref. 1 and no additional injector characterization tests were performed at these low flow rates, no inferences can be drawn concerning the quality of the spray distribution obtained during this investigation.

Test Procedure

The normal operating procedure consisted of establishing a prescribed condition (e.g., pressure, fuel and air flow rates) within the test duct and gradually increasing the inlet air temperature until autoignition occurred at the exit of the mixer/vaporizer section. It became apparent early in the program that at the planned test air flow rate of 0.05 kg/sec, long run times were required to preheat the piping which comprises the high-temperature, 20 kW heater system. In addition, at low air flow rates, unacceptably high temperatures were realized on the outer shell of the 720 kW heater. The 720 kW heater is a multipass direct contact air heater with the initial pass serving as cooling air for the outer shell. Therefore, to minimize the time required for facility heat up and to maintain the structural integrity of the 720 kW heater, an air bypass system was installed (see Fig. 1). During preheat and at all time when fuel is not being injected, the air flow was set at approximately 0.2 kg/sec. Just prior to testing, the bypass was opened and the air flow rate through the mixer/vaporizer was reduced to 0.05 kg/sec.

At temperatures above 1025K it was necessary to modify normal operating procedure because the response time of the 20 kW heater was prohibitively long. The modification included establishing a prescribed pressure, temperature and airflow rate within the test duct and gradually increasing the fuel flow rate (rather than air temperature) until autoignition occurred at the exit of the mixer/vaporizer section. Upon ignition, the test was abruptly terminated by shutting off the fuel flow, reducing the rig pressure, and purging the fuel injector with water. Subsequent tests were not performed until the system had been purged of residual fuel by the airflow which was maintained at all times. This test arrangement permitted variation of each of the important variables (i.e., pressure, temperature, velocity, residence time, and fuel-air ratio) within a fixed range of test conditions. The ignition delay time was equated to the residence time of the fuel-air mixture between the point of fuel injection and the location of the expander section (i.e., the point of autoignition). It was computed using the average flow velocity as calculated from the inlet temperature, pressure and airflow rate.

EXPERIMENTAL RESULTS AND DISCUSSION

Ignition delay tests were conducted using No. 2 diesel fuel at fuel-air equivalence ratios ranging from 0.2 to 1.0, inlet air temperatures up to 1150K and ambient pressures of 3, 4, and 5 atm. Ignition delay times in the range 6.0 msec to 60 msec were obtained by interchanging sections between the fuel injector and the expander to obtain three discrete mixer/vaporizer lengths (72.4 cm, 41.9 cm and 21.6 cm). Typically, tests were conducted at an airflow rate of 0.05 kg/sec and the resulting freestream velocities were in the range of 10 m/sec to 40 m/sec. A summary of the test results is presented in Table I.

Within the experimental accuracy, the ignition delay times for No. 2 diesel appeared to correlate with ambient pressure and inlet air temperature according to the classical Arrhenius type equation

$$\tau = A/P^n \exp(E/RT)$$

where E is the global activation energy corresponding to all the physical and chemical processes occurring during the induction period, R is the universal gas constant, and A and n are empirical constants.

Intrinsic ignition delay data require an accurate knowledge of the freestream conditions at the onset of autoignition. In the present experiment the free-stream temperature can depart from the inlet air temperature as a result of heat transferred to the fuel and to the water-cooled mixer/vaporizer wall. The temperature drop due to fuel preheating and vaporization was calculated, assuming complete vaporization and mixing. The results are presented in Fig. 4. The temperature drop due to convection was calculated using a 2-D turbulent boundary layer computer program developed at UTRC. Results indicate that centerline temperature is not affected by convection at any of the mixer/vaporizer lengths tested in the present program. Measurements of the centerline temperature drop due only to convection were made in an attempt to verify the calculation. However, quantitative verification could not be obtained by this technique because the measured temperature differences were no greater than the estimated uncertainties in the measurement (due to conduction and radiation losses and imprecise radial positioning of the thermocouple). Therefore, the calculated temperature at the onset of ignition, designated as T_{mix} in Table I, reflects the temperature loss due only to fuel preheating and vaporization.

Parametric autoignition testing of No. 2 diesel fuel was performed using the multiple conical tube injector described earlier. As expected, the results indicate that ignition delay decreases with increasing air temperature and pressure. It was determined in the previous program (Ref. 1) and confirmed in the present study that the ignition delay times appear to correlate best with the inverse square of pressure and the inverse exponent of temperature. Therefore ignition delay data are plotted in Fig. 5 as the product of delay time and the square of pressure (τP^2) versus the reciprocal of inlet air temperature. For completeness, data obtained at mixer/vaporizer lengths greater than 22 cm in Ref. 1 are also shown in the figure. Although high-performance gas turbine engines would require shorter premixing lengths, the results of tests performed in Ref. 1 at shorter mixer/vaporizer lengths are not included in the figure since it was concluded that mixture nonuniformities, such as would be obtained at short lengths, tended to increase the likelihood of autoignition and resulted in a shifting of the data.

The data in Fig. 5, represented by the solid and open symbols, correspond to large differences in the fuel and air flow rates. These differences may affect the performance of the fuel injector, causing differences in the spray characteristics (i.e., droplet size and distribution) which could affect the magnitude of the ignition delay. However, as stated previously, injector characterization tests to experimentally substantiate this hypothesis were beyond the scope of the present effort. The absence of spray data notwithstanding, the results indicate a definite decrease in the slope of the ignition delay curve (i.e., a decrease in the global activation energy) as temperature increases. The trend to decreasing global activation energy with increasing inlet air temperature has been reported by a number of other investigators

(e.g., Refs. 1, 3, 4, 5 and 6) and may reflect a change in the relative importance of the constituent processes (i.e., chemical reaction vs. physical delay) or a change in the nature of the chemical reaction occurring. That is, at short residence times the relative importance of atomization, vaporization and mixing is increased compared to the times associated with reaction kinetics. Also, the specific reaction mechanism and the relative importance of particular reactions are probably temperature dependent.

Finally, because it was necessary to ramp the fuel flow rate, it was not possible to obtain sufficient data at specific fuel-air equivalence ratios to conclusively determine whether or not there is any effect of equivalence ratio on autoignition. The data obtained in Ref. 1 indicated that ignition delay times decreased with increasing equivalence ratios, particularly at equivalence ratios between 0.3 and 0.5.

In Fig. 6 the ignition delay times determined for No. 2 diesel are compared with ignition delays measured by other investigators for typical gas turbine fuels. The data of previous investigators were correlated in Ref. 7, according to the Arrhenius equation, using a pressure exponent equal to unity ($n = 1.0$). Therefore, in order to permit direct comparisons of results, the present data and the data of Ref. 1 were correlated with a pressure exponent of unity. The figure shows that there is general agreement of the data. Differences between the present and previous studies are the degree of mixing, extent of vaporization achieved and, to a lesser extent, the types of fuels tested. In most of the previous studies shown, the ignition delay curves exhibit a decreasing slope with increasing temperature (i.e., decreasing residence time). As discussed above, at high air temperatures, the time required for formation of a combustible mixture can represent a significant percentage of the ignition delay time. Since this limitation is intrinsic in all of the data shown in Fig. 6, albeit at a unique set of operating conditions for each apparatus, careful consideration of both the test apparatus and the operating conditions is required when interpreting autoignition data.

CONCLUDING REMARKS

The ignition delay characteristics of No. 2 diesel fuel in air have been investigated over a range of inlet air temperatures and pressures representative of regenerative-cycle automotive gas turbine engines. The data obtained appear to be in agreement with data obtained earlier and behave in a predictable manner; that is, ignition delay time decreased with increasing temperature and pressure.

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TABLE I

IGNITION DELAY OF NO. 2 DIESEL FUEL

| L | P | T _{air} | T _{mix} | Airflow Rate | Fuel Flow Rate | V _{air} | Equivalence Ratio | Ignition Delay |
|------|-----|------------------|------------------|-----------------|-------------------|------------------|----------------------|----------------------------|
| cm | atm | K | K | kg/sec | kg/sec | m/sec | | secx10 ³ |
| 72.4 | 5.0 | 792 | 700 | .038 | .00305 | 11.9 | 1.18 | 60.9 |
| 72.4 | 5.0 | 878 | 857 | .049 | .00067 | 17.0 | 0.20 | 42.7 |
| 72.4 | 5.0 | 868 | 818 | .043 | .00155 | 14.7 | 0.53 | 49.1 |
| 72.4 | 4.9 | 815 | 738 | .038 | .00233 | 12.4 | 0.90 | 58.4 |
| 72.4 | 4.9 | 876 | 843 | .048 | .00104 | 16.7 | 0.32 | 43.3 |
| 72.4 | 3.1 | 953 | 856 | .049 | .00313 | 29.5 | 0.94 | 24.6 |
| 72.4 | 3.1 | 971 | 898 | .051 | .00236 | 31.0 | 0.68 | 23.4 |
| 72.4 | 3.1 | 1009 | 956 | .050 | .00156 | 31.2 | 0.46 | 23.2 |
| 72.4 | 3.1 | 1012 | 974 | .049 | .00103 | 31.1 | 0.31 | 23.3 |
| 72.4 | 3.1 | 1020 | 992 | .048 | .00072 | 31.2 | 0.22 | 23.1 |
| 41.9 | 5.1 | 1014 | 975 | .041 | .00103 | 16.1 | 0.37 | 26.0 |
| 41.9 | 5.1 | 1017 | 984 | .040 | .00060 | 15.5 | 0.22 | 27.0 |
| 41.9 | 5.0 | 1001 | 948 | .045 | .00156 | 17.8 | 0.51 | 23.5 |
| 41.9 | 4.9 | 993 | 897 | .049 | .00313 | 19.6 | 0.94 | 21.4 |
| 41.9 | 4.1 | 1069 | 967 | .049 | .00310 | 25.1 | 0.93 | 16.7 |
| 41.9 | 4.0 | 1078 | 968 | .044 | .00308 | 23.4 | 1.03 | 17.9 |
| 41.9 | 4.0 | 1105 | 1048 | .046 | .00153 | 24.6 | 0.49 | 17.0 |
| 41.9 | 3.9 | 1079 | 970 | .047 | .00310 | 25.2 | 0.97 | 16.6 |
| 41.9 | 3.9 | 1093 | 973 | .045 | .00309 | 24.4 | 1.01 | 17.2 |
| 41.9 | 3.9 | 1107 | 1068 | .045 | .00100 | 24.8 | 0.33 | 16.9 |
| 41.9 | 3.9 | 1110 | 1079 | .045 | .00080 | 24.9 | 0.26 | 16.9 |
| 41.9 | 3.9 | 1111 | 1000 | .042 | .00271 | 23.3 | 0.94 | 18.0 |
| 41.9 | 3.8 | 1114 | 1049 | .041 | .00153 | 23.2 | 0.55 | 18.0 |
| 41.9 | 3.7 | 1103 | 1063 | .066 | .00242 | 39.4 | 0.54 | 10.6 |
| 41.9 | 3.1 | 1142 | 1057 | .057 | .00271 | 41.2 | 0.70 | 10.2 |
| 41.9 | 3.1 | 1144 | 1059 | .047 | .00271 | 41.5 | 0.70 | 10.1 |
| 41.9 | 3.1 | 1144 | 1091 | .057 | .00171 | 41.4 | 0.49 | 10.1 |
| 41.9 | 3.1 | 1147 | 1119 | .057 | .00089 | 41.6 | 0.23 | 10.1 |
| 41.9 | 3.1 | 1125 | 1058 | .058 | .00221 | 40.9 | 0.56 | >10.3 No auto- ignition |
| 21.6 | 4.7 | 1117 | 1052 | .047 | .00213 | 27.0 | 0.35 | 9.0 |
| 21.6 | 4.2 | 1102 | 993 | .039 | .00252 | 20.2 | 0.95 | 10.7 |
| 21.6 | 4.1 | 1117 | 1013 | .042 | .00251 | 22.4 | 0.88 | 9.6 |
| 21.6 | 3.9 | 1117 | 1050 | .051 | .00198 | 28.3 | 0.57 | 7.6 |
| 21.6 | 3.9 | 1110 | 1061 | .046 | .00241 | 20.0 | 0.77 | 10.8 |
| 21.6 | 3.8 | 1113 | 1085 | .049 | .00080 | 28.0 | 0.24 | 7.7 |
| 21.6 | 3.2 | 1127 | 1017 | .052 | .00325 | 35.7 | 0.92 | 6.0 |
| 21.6 | 3.5 | 1146 | 1064 | .066 | .00328 | 42.0 | 0.73 | >5.0 No auto- ignition |

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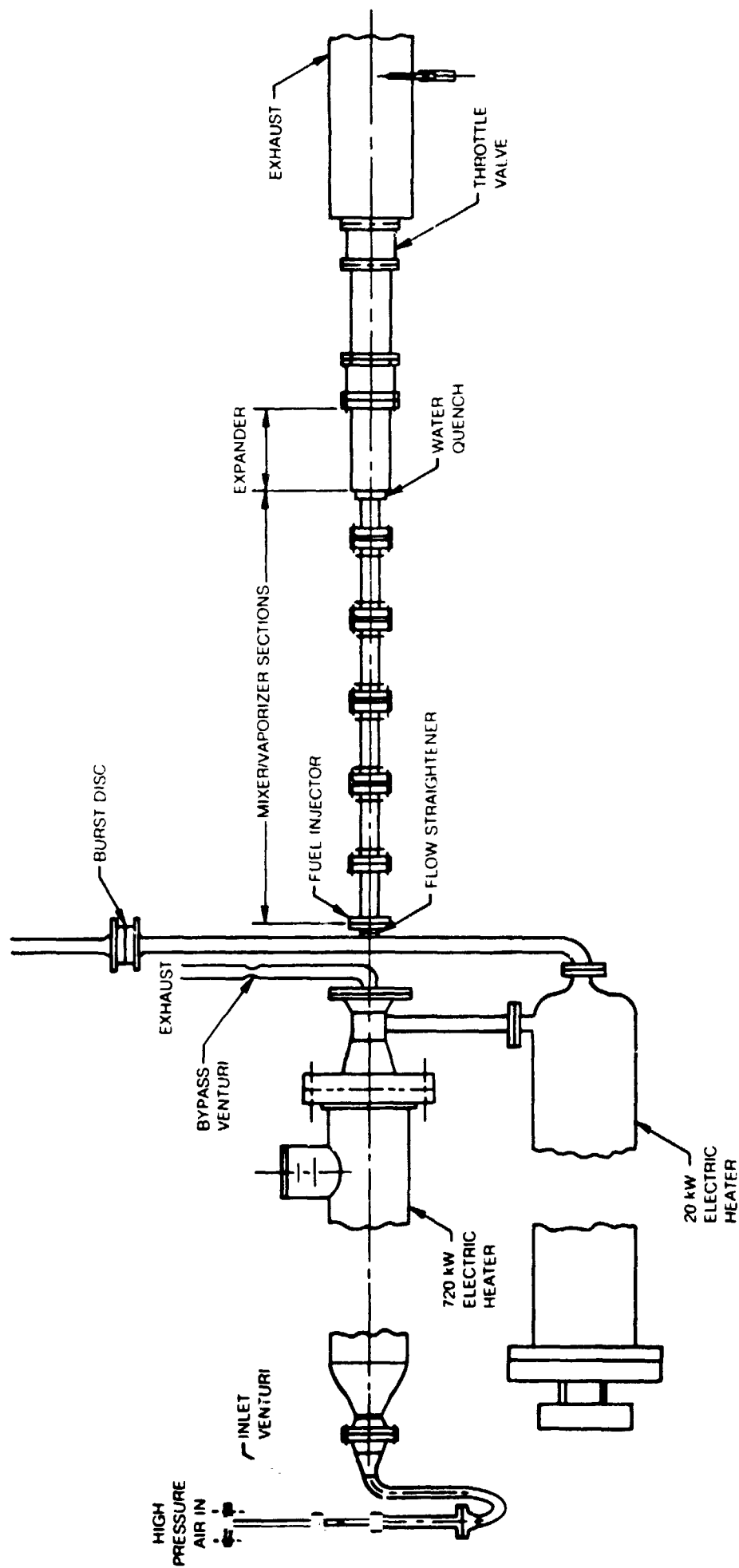


Figure 1 Autoignition Test Assembly

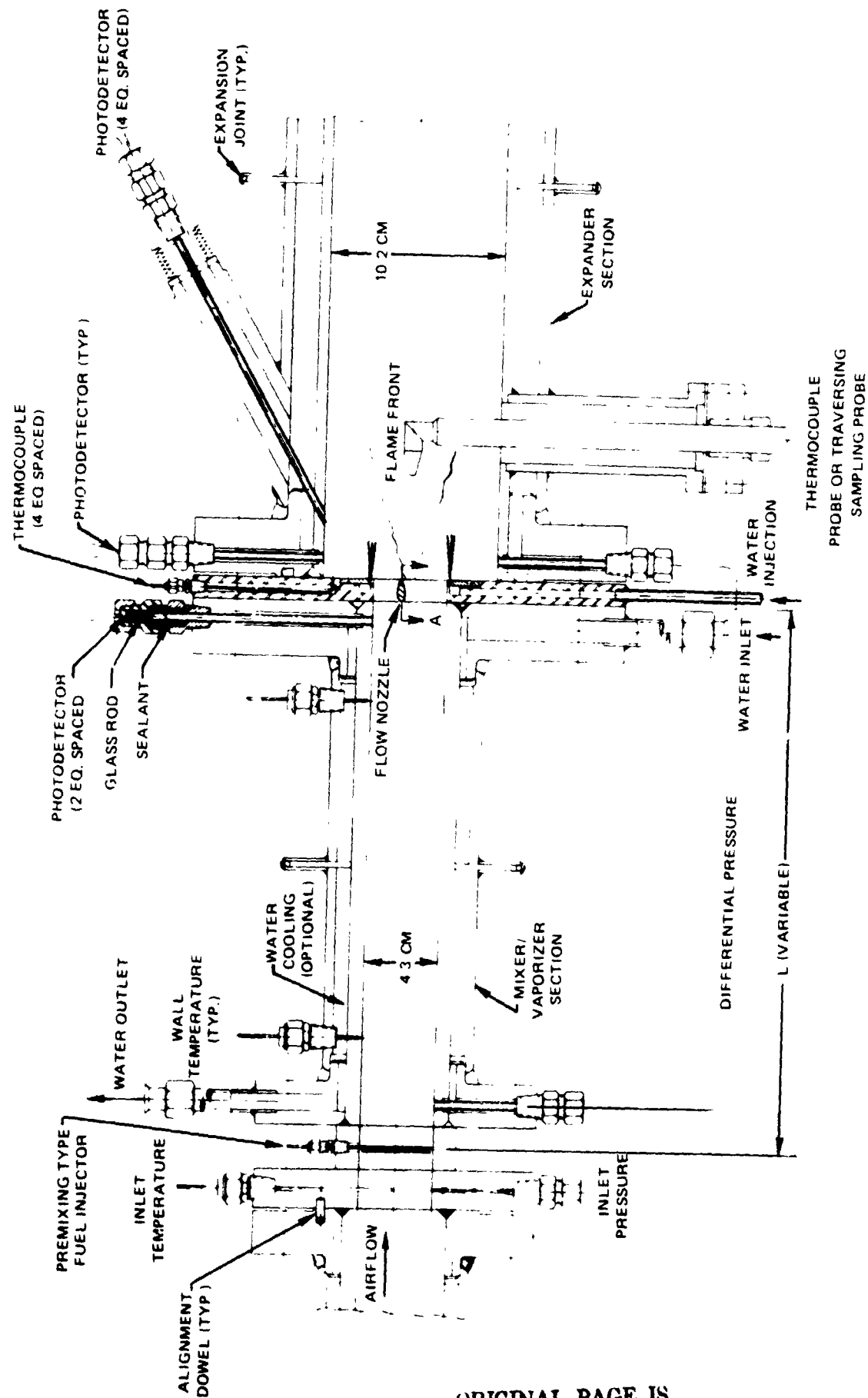


Figure 2 Mixer/Vaporizer and Expander Assembly

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BLOCKAGE = 70 PERCENT
ALL DIMENSIONS IN CM

FUEL INLET TUBE
0.084 ID

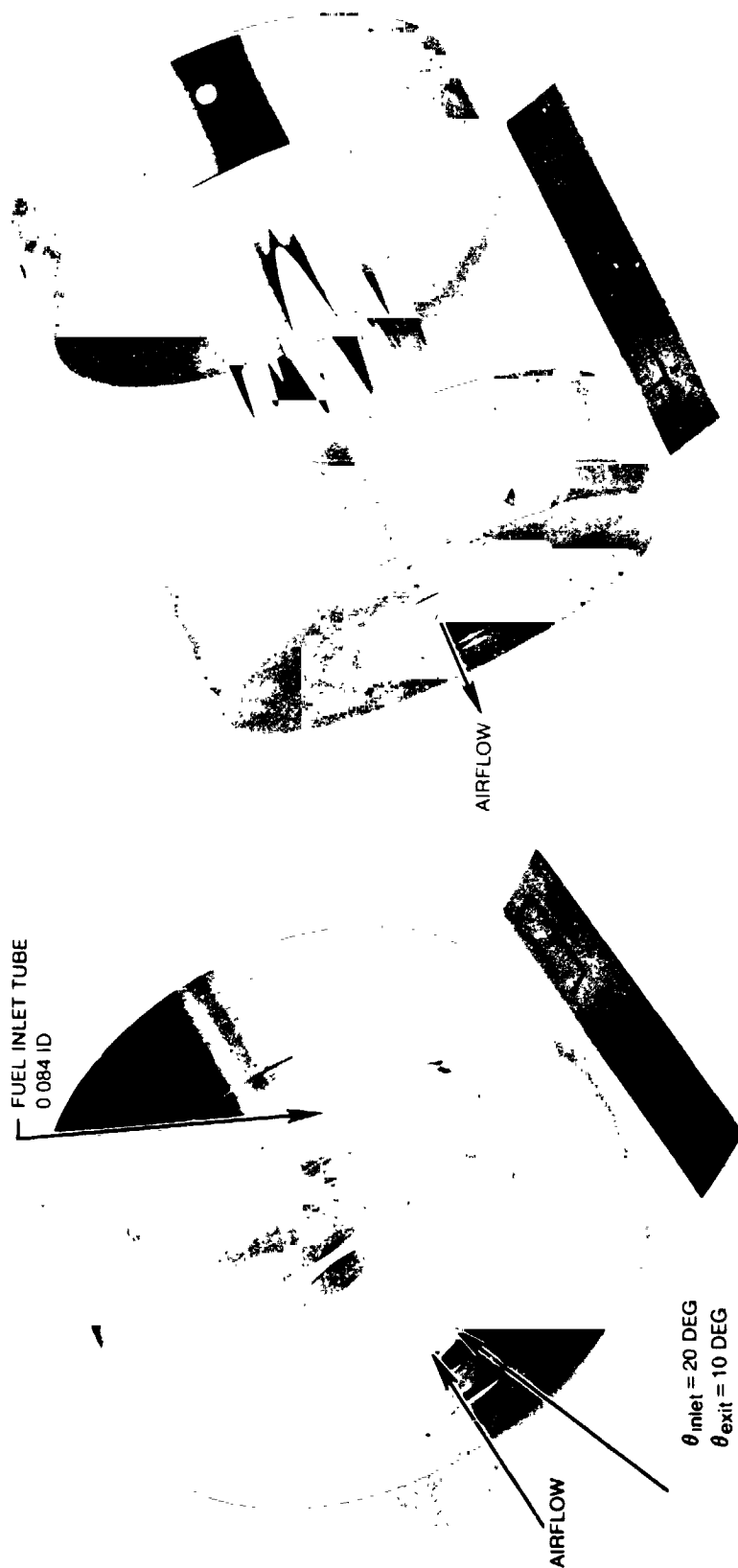


Figure 3 Multiple Conical Tube Costream Injector

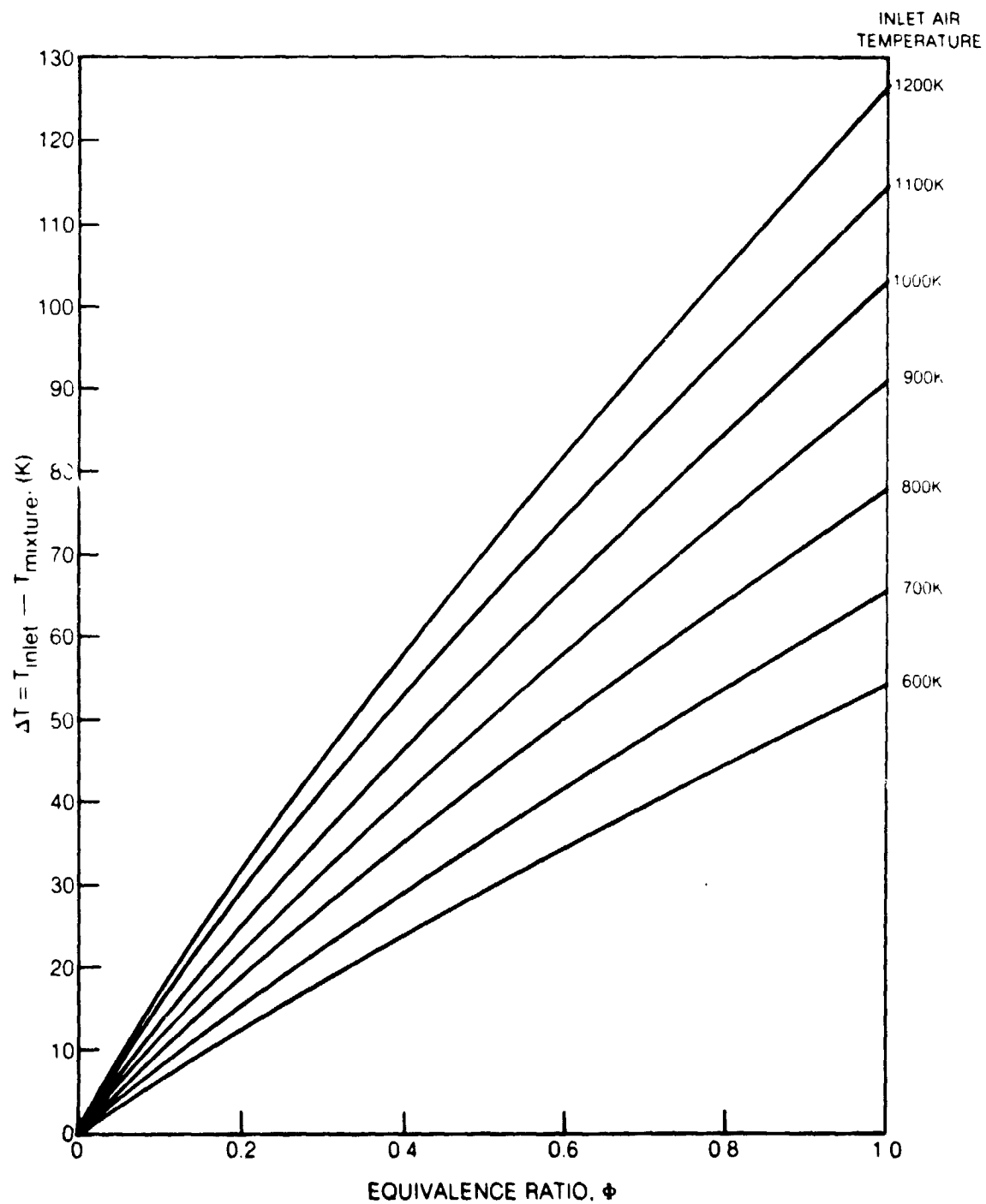


Figure 4 Airstream Cooling Due to Fuel Vaporization

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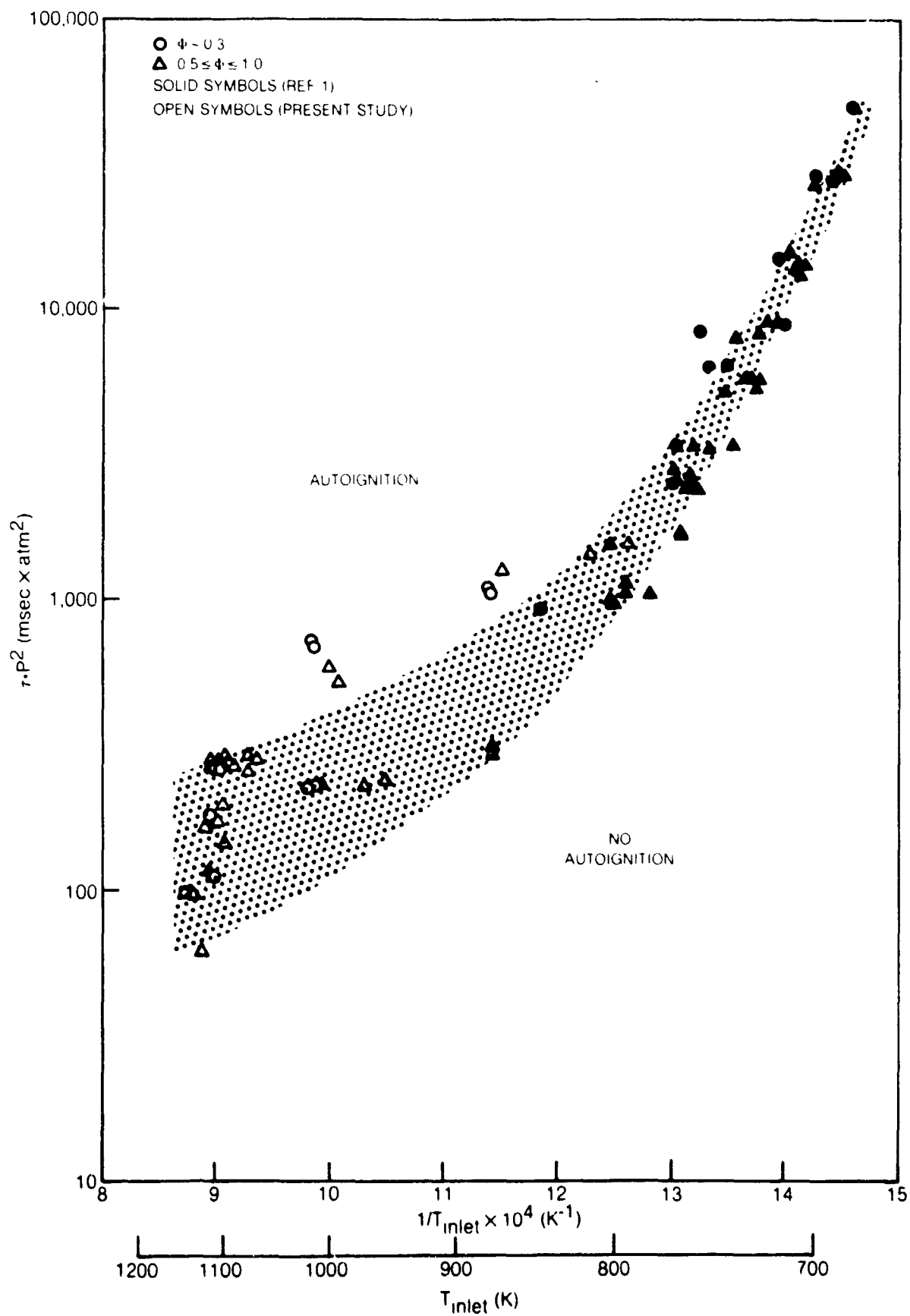


Figure 5 Autoignition Characteristics of No. 2 Diesel Fuel in Air

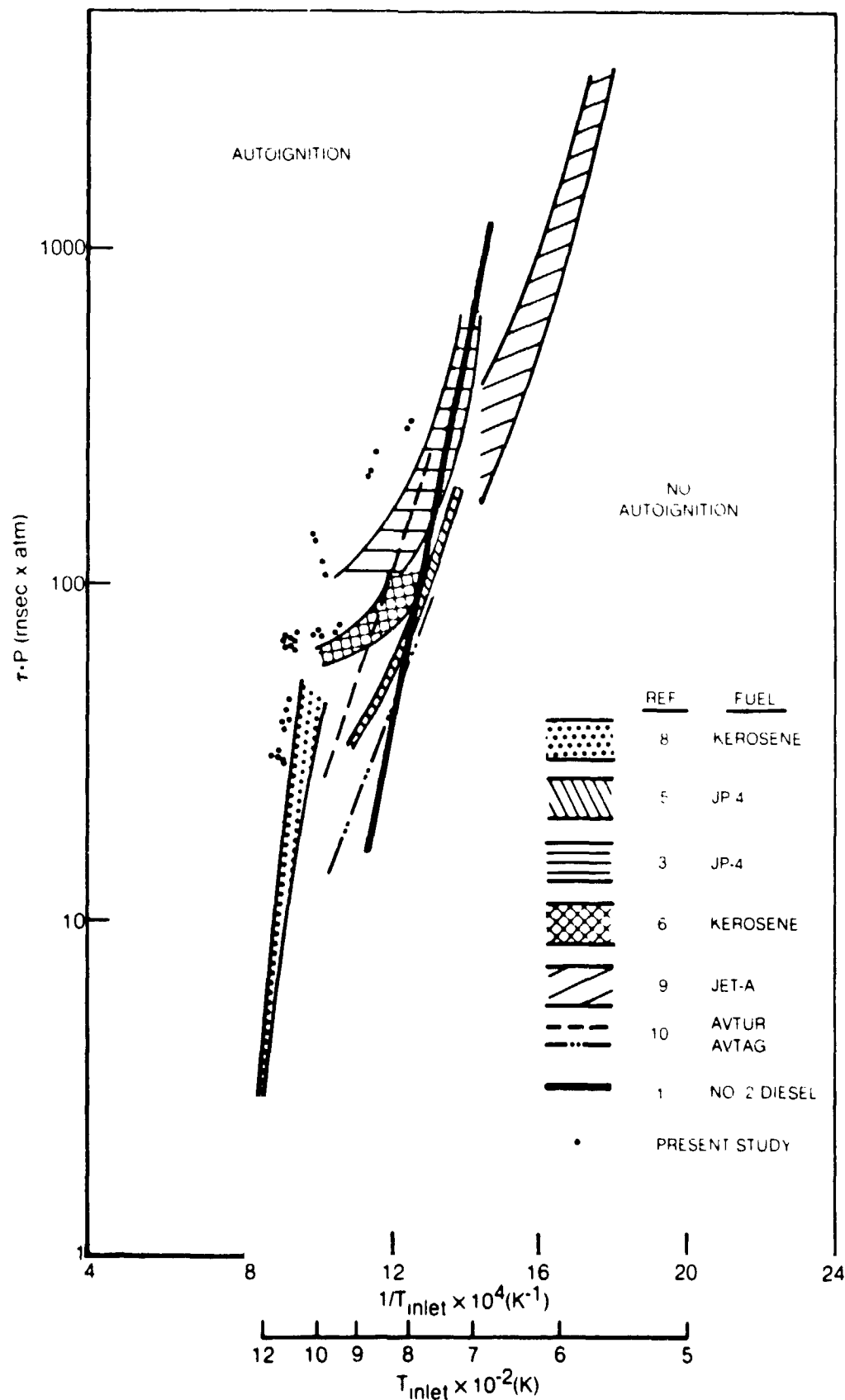


Figure 6 Autoignition of Liquid Hydrocarbon Fuel Sprays in Air (Ref. 7)

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| 16. Abstract An applied research program was undertaken to evaluate the autoignition characteristics of No. 2 diesel fuel in air at inlet temperatures of up to 1150K, pressures of 3, 4 and 5 atm, and fuel-air equivalence ratios ranging from 0.2 to 1.0. Ignition delay times in the range of 6 to 60 msec at freestream flow velocities ranging from 10 to 40 m/sec were obtained using a continuous flow test apparatus which enabled the independent variation and evaluation of the effects of temperature and pressure on the ignition delay. The ignition delay times were correlated with the inverse of pressure and inverse exponent of temperature, viz; $\tau = \frac{A}{p^n} \exp (E/RT)$ | | | |
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